PROGRESS ON OPTIMIZATION OF THE SOLAR CELL FABRICATION PROCESS BY IMPURITY-TO-EFFICIENCY PREDICTIVE SIMULATOR

Ana Peral, Carlos del Cañizo and Antonio Luque

Instituto de Energía Solar, Universidad Politécnica de Madrid
ETSI Telecomunicación, Avda. Complutense, 30, 28040 Madrid, Spain

ABSTRACT: To optimize the last high temperature step of a standard solar cell fabrication process (the contact co-firing step), the aluminium gettering is incorporated in the Impurity-to-Efficiency simulation tool, so that it models the phosphorus and aluminium co-gettering effect on iron impurities. The impact of iron on the cell efficiency will depend on the balance between precipitate dissolution and gettering. Gettering efficiency is similar in a wide range of peak temperatures (600-850 ºC), so that this peak temperature can be optimized favoring other parameters (e.g. ohmic contact). An industrial co-firing step can enhance the co-gettering effect by adding a temperature plateau after the peak of temperature. For highly contaminated materials, a short plateau (< 2 min) at low temperature (600 ºC) is shown to reduce the dissolved iron.
Keywords: aluminum gettering; co-firing; modeling

1 INTRODUCTION

Through the high temperature steps during the solar cell fabrication process, some metal impurities vary their concentration and distribution within the silicon material. Then, their detrimental effect on the material quality is modified. In particular, iron role is very relevant, being a dominant metal impurity in silicon solar cells[1].

Iron kinetic behavior has been widely investigated for two high temperature steps of the wafer and solar cell fabrication process, crystallization and phosphorus emitter diffusion. Solid-liquid iron segregation during crystallization has been observed to purify silicon in a 2 to 3 order of magnitude [2,3], and iron segregation to the phosphorus highly doped layer during emitter diffusion has been used for enhancing material quality by defect engineering tools such as the phosphorus diffusion gettering (PDG) and the so-called extended gettering [4,5,6].

The high temperature step at the end of the solar cell fabrication process, the contact co-firing step, has been observed to have an effect on interstitial iron concentration [Fe_i] [7,8] that can be explained by the competing phenomena of dissolution and gettering [9]. A defect engineering tool named extended contact co-firing has been proposed, based in the final [Fe_i] reduction by enhancing phosphorus gettering [10]. The following step is to include the aluminium gettering effect that is present in combination with the phosphorus gettering during this last process step.

To help in process optimization, the simulation tool called "Impurity-to-Efficiency" (I2E) developed by Hofstetter *et al.* [11] predicts final solar cell performance taking as inputs the initial material quality, in terms of iron distribution and concentration, and the processing conditions. The model takes into account the iron diffusion, the dissolution and growth of iron silicide precipitates and the segregation of iron to a diffused phosphorus layer.

The objective of this work is to study the aluminium-phosphorus co-gettering effect on interstitial iron concentration [Fe_i], during the industrial contact co-firing step. First, the aluminum gettering effect is incorporated in the I2E simulation tool. Second, the effect of aluminium and phosphorus co-gettering on [Fe_i] is simulated. Finally, the co-gettering dependence on the initial material contamination level, i.e. initial iron concentration and distribution, is studied.

2 APPROACH

2.1 Model innovations description: Phosphorus and aluminium co-gettering

Our simulation model Impurity-to-Efficiency is complemented with the incorporation of the iron segregation to an aluminium silicon alloy layer. In this manuscript the changes related to the kinetics of iron are described. The rest of physics, assumptions, and validations are detailed in Hofstetter *et al.* [11].

To describe the kinetics of iron atoms within the silicon, the interstitial iron concentration $[\mathrm{Fe_i}](x,t)$, is modeled along the wafer thickness, x, as a function of processing time, t, using a finite element mesh. The model uses the diffusion-segregation equation by Tan *et al.*[12] modified to contain two segregation components:

$$\frac{\partial[\mathrm{Fe_i}]}{\partial t} = \frac{\partial}{\partial x}\left[D_{Fe}\left(\frac{\partial[\mathrm{Fe_i}]}{\partial x} - \frac{[\mathrm{Fe_i}]}{\sigma_1}\frac{\partial \sigma_1}{\partial x} - \frac{[\mathrm{Fe_i}]}{\sigma_2}\frac{\partial \sigma_2}{\partial x}\right)\right] \quad (1)$$

The first term represents Fick's law of diffusion with a temperature-dependent diffusion coefficient of iron in silicon D_{Fe}. The second term is related to the iron segregation to the phosphorus layer with a space-temperature-dependent segregation coefficient $\sigma_1(x)$, described by Haarahiltunen *et al.*[13]. The third term incorporates the iron segregation effect to the aluminium-silicon layer with the space-temperature-dependent segregation coefficient $\sigma_2(x)$. This coefficient described by Tan *et al.* [12] takes the value of 1 in Si, while in the Al-Si liquid its value S depends exponentially on the temperature. It has been experimentally measured ~~between 950-110 ºC~~by Abdelbarey *et al.*[14]:

$$S = 0.056 \cdot \exp^{\left(\frac{1.59}{kT}\right)} \quad (2)$$

where k is the Boltzmann constant.

2.2 Simulation scenario

The phosphorus-aluminum gettering effect during the contact co-firing step has been simulated with the help of the model I2E.

The material defined as input in the simulations is a

silicon substrate with a phosphorus emitter on the front side and an aluminum layer on the rear. The silicon nitride layer and the front metal pastes are supposed to have no effect on the iron dynamics. The interstitial iron concentration [Fe_i] before the firing step is assumed to be $5 \cdot 10^{11}$ cm^{-3} for all the cases.

The [Fe_i] after the co-firing step is obtained by the simulation. The effects of three types of industrial co-firing step are studied. The first temperature profile simulated is the standard co-firing, consisting of an annealing at the temperature peak (the general case is 850 ºC) during 10 s followed by a fast cool down to room temperature (see black line in Figure 1). The next two profiles are a variation of the standard co-firing, called "extended co-firing", and proposed successfully in previous simulations and laboratory experiments [10, 14]. It consists of an annealing at the peak temperature during 10 s followed by a temperature plateau at 730 ºC and a fast cool-down to room temperature. This temperature plateau has a length of 100 s and 300 s, respectively (see blue and grey lines in Figure 1).

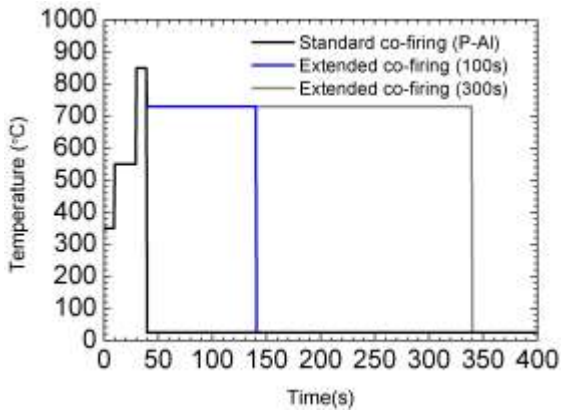


Figure 1: Standard and extended contact co-firing temperature profiles used for the simulations.

3 SIMULATION RESULTS AND DISCUSSION

3.1 Temperature peak of contact co-firing

To know the effect of aluminium and phosphorus co-gettering on [Fe_i] during a standard co-firing step at different temperature peaks, varying between 600 and 950 ºC, we simulate the final [Fe_i] without gettering layers (black line in Figure 2), with only phosphorus gettering (blue line in Figure 2), and with both aluminium and phosphorus co-gettering effects (grey line in Figure 2).

As I2E input parameters, an initial total iron concentration $[Fe_{total}]_0 = 5 \cdot 10^{14}$ cm^{-3} and an initial precipitate radius $r_0 = 30$ nm are assumed. Figure 2 shows the final [Fe_i] as a result of the contact co-firing step at different peak temperatures for the three gettering scenarios.

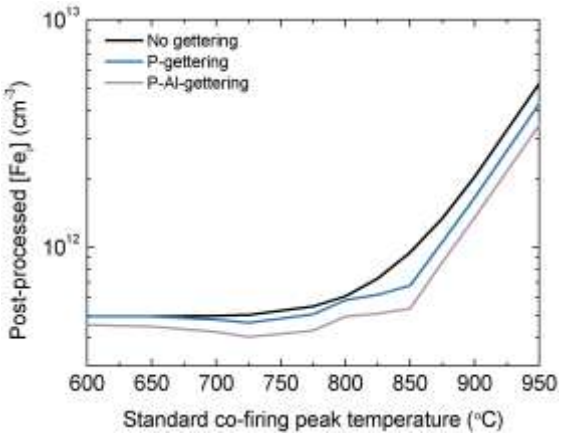


Figure 2: Final interstitial iron concentration, [Fe_i], after a contact co-firing step varying the peak temperature.

The simulation results show that the short annealing at high temperature during only 10 seconds can reduce the final [Fe_i] by phosphorus-aluminium co-gettering.

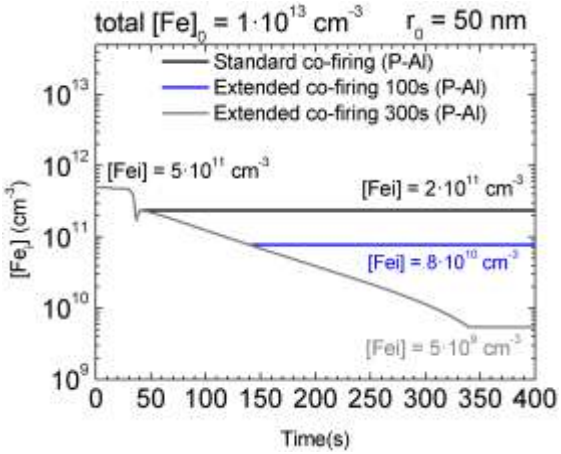
In addition, multiple solutions are found for contact co-firing peak temperature optimization. Gettering is similar in a wide range of peak temperatures (600-850 ºC), so that other parameters can be optimized without affecting the gettering effect (i.e., the ohmic contact or the pastes penetration rate).

3.2 Final interstitial iron concentration dependence on initial material: low contamination level materials

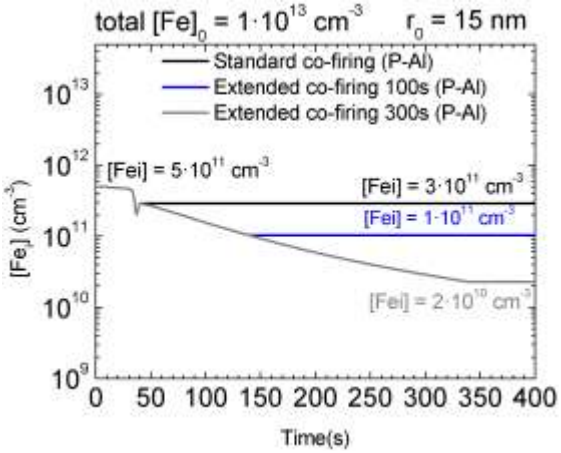
To study the co-gettering effect dependence on initial material, [Fe_i] evolution during the co-firing step is firstly simulated for materials with a low initial total Fe concentration ($[Fe_{total}]_0 = 1 \cdot 10^{13}$ cm^{-3}). Figure 3(a) show [Fe_i] evolution for material containing big precipitates (initial r_0 = 50 nm) and Figure 3 (b) for material containing little precipitates (initial r_0 = 15 nm). Both materials are simulated to be processed with the three type of co-firing.

Some conclusions can be extracted from the simulations:

- extended co-firing is able to reduce the final [Fe_i] as compared to the previous value because the gettering effect ([Fe_i] decrease) is enhanced with respect to the dissolution of precipitates ([Fe_i] increase);
- a long plateau is more beneficial than a short one because precipitate dissolution rate is lower than segregation effect and then the [Fe_i] decreases with time;
- smaller precipitates material has a higher final [Fe_i] because little precipitates dissolve faster [15] and the gettering is the same in the two cases.



(a)



(b)

Figure 3: Low level of contamination initial materials containing big (a) and little (b) silicide precipitates

3.3 Final interstitial iron concentration dependence on initial material: high contamination level materials

We have also simulated [Fe_i] evolution during the co-firing step for materials with a high initial total Fe concentration ([Fe_{total}]$_0$ = $5\cdot10^{15}$ cm^{-3}). Figure 4 (a) shows [Fe_i] evolution for a material containing big precipitates (initial r_0 = 50 nm) and Figure 4(b) for a material containing little precipitates (initialr_0 = 15 nm). Both materials are simulated to be processed with the three type of co-firing. In addition, a contact co-firing step with a plateau at low temperature (600ºC) during 300 seconds has been simulated for little precipitates (see red line of the Figure 4(b)). Some conclusions can be observed from the simulations:

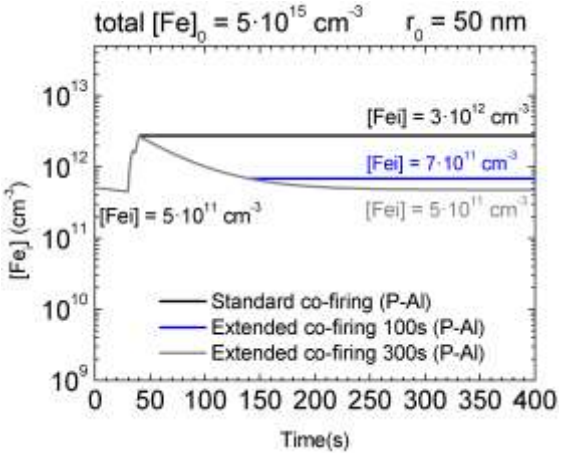
-the standard contact co-firing has a detrimental effect by increasing the final [Fe_i] well above the initial value;

-the extended co-firing has a beneficial effect by reducing the [Fe_i];

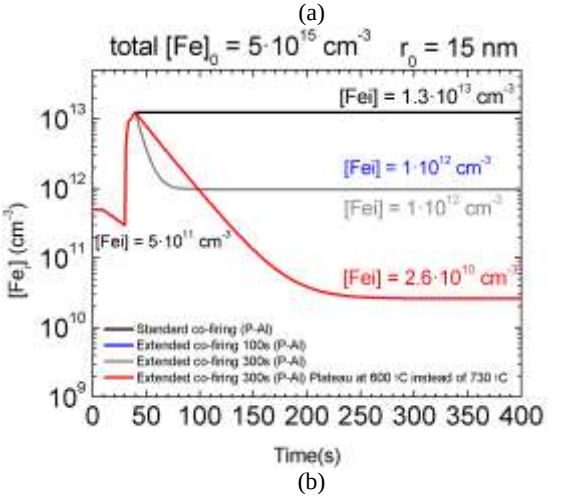
-an equilibrium [Fe_i] is reached because dissolution and gettering are competing and during this equilibrium [Fe_{total}] is decreasing;

-reducing the time of the plateau with high contaminated materials allows to reach the same final [Fe_i];

-to reduce final [Fe_i] maintaining the process duration, it is necessary to decrease the plateau temperature to increase the segregation and decrease the dissolution.



(a)



(b)

Figure 4: High level of contamination initial materials containing big (a) and little (b) silicide precipitates

Comparing with the low contaminated materials, the final [Fe_i] is greater for the highly contaminated ones due to the fact that dissolution is higher and the segregation is the same in both cases. Precipitates can dissolve to an upper limit given by the solid solubility of Fe in silicon ($1.2\cdot10^{12}$ cm^{-3} at 730ºC). It can be observed that the dissolved iron during the plateau for thehigh contamination level is $5\cdot10^{11}$-$1\cdot10^{12}$$cm^{-3}$, very near to the maximum.

4 CONCLUSIONS

I2E simulation tool is now more realistic by incorporating the aluminium gettering effect. This work has shown through simulations that contact co-firing peak temperature can be chosen in a wide range without affecting the gettering effect importantly. A beneficial effect of an industrial compatible optimized temperature profile ("extended contact co-firing") that reduces the possible detrimental effect of this last step has been shown. For highly contaminated wafers, adding a short time and low temperature plateau is enough to produce an enhanced gettering effect.

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